Scientific Annals of Computer Science vol. 35 (1), 2025, pp. 87–122
doi: 10.47743/SACS.2025.1.87

Degree-Based and Neighborhood Degree Sum-Based Entropy Measure of Molnupiravir

Shibsankar Das[1,2], Arti Kumari[3] and Jayjit Barman[4]

Abstract

An entirely novel virus that causes severe acute respiratory syndrome began to spread around the world at the end of 2019. Since there are no curative treatments to treat the viral infection, efforts are being made globally to stop the coronavirus from spreading. The coronavirus strain is also known as 2019-nCoV and officially identified as SARS-CoV-2 (severe acute respiratory syndrome coronavirus 2). Several distinctive characteristics of graphs have been used to differentiate the construction of entropy-based measurements from the structure of chemical graphs. Graph entropies have emerged as the information-theoretic quantities for quantifying the fundamental information of chemical graphs. The prospective applicability of the graph entropy measure in discrete mathematics, biology and chemistry has drawn attention from the scientific community. In this work, we study the structural properties of one of the known antiviral drugs, Molnupiravir, and introduce the concept of entropy measure for this drug. We evaluate the degree-based and neighborhood degree sum-based entropy by considering the values of topological indices of the chemical

This work is licensed under the Creative Commons Attribution Licence (CC BY)

[1]Corresponding author.

[2]Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India, Emails: shibsankar@bhu.ac.in, shib.cgt@gmail.com

[3]Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India, Email: ak0891497@gmail.com

[4]Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India, Email: jayjit44@bhu.ac.in

compound. Furthermore, we present the graphical representations of these entropy measures. A comparative analysis of degree-based and neighborhood degree sum-based topological indices, along with their associated entropy measures, is presented for Molnupiravir through graphical illustrations using numerical data.

Keywords: Topological index; Entropy measures; Molnupiravir; SARS-CoV-2.

1 Introduction

Mathematics-based chemical analysis is known as mathematical chemistry. A subfield of mathematical chemistry that merges chemistry and mathematics by using graph theory is known as chemical graph theory (CGT). In CGT, a molecular graph is used to carry out a topological illustration of a molecule to correlate the chemical structure with different physical attributes, chemical reactivity, or biological activity. Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ represent a molecular graph with an edge set $E(\Upsilon)$ and a vertex set $V(\Upsilon)$. When w_1 and w_2 are two adjacent vertices of Υ, the edge that joins them is denoted by w_1w_2. The *degree* (or the number of its first neighbors) of vertex w_1 in graph Υ is indicated by the symbol $deg(w_1)$. For any vertex w_1, the value of $\tau(w_1) = \{\sum_{w_2 \in V(\Upsilon)} deg(w_2) : e = w_1w_2 \in E(\Upsilon)\}$ represents the *neighborhood degree sum* of the vertex w_1 [28]. The graph-invariant quantity obtained from a graph representing a molecule is called a *topological index*. It demonstrates a relationship to the chemical constitution and shows how various chemical, physical, and biological aspects correlate with chemical structure [27].

In 1948, Shannon initially developed the concept of entropy in his well-known study [21], stating "The entropy of a probability distribution is known as a measure of the unpredictability of information content or a measureDegree-Based and Neighborhood Degree Sum-Based Entropy Measures of Molnupiravir of the uncertainty of a system". Subsequently, the study of entropy has found an extensive application in determining the structural information of graphs / chemical structures / networks. As Rashevsky developed the graph entropy concept in 1955 which was based on the categorization of vertex orbits [20]. These days, the significance of graph entropies has risen substantially in multiple disciplines, such as biology, sociology, ecology, computer science, structural chemistry and mathematics. The previously mentioned graph entropy measures are a broad category that can be classified as intrinsic and extrinsic measures. They are defined to correlate the probability distributions with graph elements

(vertices, edges, etc.). Dehmer explored the information functionals based graph entropies, which analyze the characteristics of structural information and capture it [9,10]. Entropic network measures have broad applications, ranging from software technology or quantitative structural description in structural chemistry to studying chemical or biological features of molecular graphs. We highlight that the applications previously described have to do with resolving an underlying data analysis issue, for example: classification tasks or clustering. Although it is ambiguous on which graph category the measure should be assessed, the task is complex. We speculate that network heterogeneity can be measured using the introduced degree-based entropy. Now, we discuss some important research articles on degree-based graph entropy measures that have shown their importance and applicability in literature. Recently, Li et al. investigated the analysis of entropy measures for titanium dioxide via rational curve fitting methods in [18]. Manzoor et al. worked on entropy measures of polycyclic hydroxychloroquine used for novel coronavirus (COVID-19) treatment in [19]. In 2023, Hussain et al. shown interest on K-Banhatti indices and entropy measure for rhodium (III) chloride via linear regression models in the article [1]. Srinivasan et al. [23] created Lakvir indices, a new class of vertex degree-based topological indices, and investigated how to derive them using Lakvir M-Polynomials (LM Polynomials) for specific medications used to treat Omicron and COVID-19. Tamilarasi et al. [24] created the QSPR model to forecast a few specific physicochemical properties and ADMET properties of the COVID-19 Omicron drugs by using some degree-based indices such as the first K Banhatti index, second K Banhatti index, first K hyper Banhatti index, second K hyper Banhatti index, modified first K Banhatti index, modified second K Banhatti index and harmonic K Banhatti index via M-Polynomial. In the article [3], Chu et al. present an efficient edge-partition-based approach for computing degree-based and irregularity-based topological descriptors of two benzenoid structures, enabling cost-effective theoretical prediction of compound properties via QSAR and QSPR analyses. Julietraja et al. [13] computed neighborhood sum degree-based indices for sodalite structures to reveal how molecular structure influences physical properties through derived descriptors. Julietraja et al. [14] derive analytical expressions for degree-based entropy measures in three key classes of coronene-centered polycyclic aromatic hydrocarbons, revealing structural insights through entropy-molecular relationships.

Edge-Weight-Based Entropy of a Graph

Chen et al. [2] defined the entropy of an edge-weighted graph for the first time in 2014. Suppose that $\Upsilon = (V(\Upsilon), E(\Upsilon), \phi(w_1w_2))$ represented as an edge-weight graph, where $V(\Upsilon), E(\Upsilon)$ and $\phi(w_1w_2)$ stands for the vertex set, edge set and the edge-weight of an edge $w_1w_2 \in E(\Upsilon)$. Therefore, the entropy of an edge-weight graph is represented as follows:

$$E_\phi(\Upsilon) = -\sum_{w_1'w_2' \in E(\Upsilon)} \frac{\phi(w_1'w_2')}{\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)} \log\left(\frac{\phi(w_1'w_2')}{\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)}\right). \quad (1)$$

Equation 1 can be simplified to Equation 2 by following these steps:

$$\begin{aligned}
E_\phi(\Upsilon) &= -\sum_{w_1'w_2' \in E(\Upsilon)} \frac{\phi(w_1'w_2')}{\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)} \Bigg[\log\left(\phi(w_1'w_2')\right) \\
&\quad - \log\Big(\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)\Big)\Bigg] \\
\implies E_\phi(\Upsilon) &= \log\Big(\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)\Big) \\
&\quad - \sum_{w_1'w_2' \in E(\Upsilon)} \frac{\phi(w_1'w_2')}{\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)} \log\left(\phi(w_1'w_2')\right) \\
\implies E_\phi(\Upsilon) &= \log\Big(\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)\Big) \\
&\quad - \frac{1}{\Big(\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2)\Big)} \sum_{w_1'w_2' \in E(\Upsilon)} \phi(w_1'w_2') \log\left(\phi(w_1'w_2')\right).
\end{aligned} \quad (2)$$

Motivation and Methodology

Broadly seeing the application of entropy measures in several fields, the degree-based and neighborhood degree sum-based entropy measures are utilized to quantify the complexity and diversity of molecules. In the realm of drug design, these entropies can be beneficial for identifying compounds with desired features during the screening and analysis of molecular graphs and for enhancing the molecular descriptors for QSAR/QSPR models. Recently, the

work on degree-based and neighborhood degree sum-based entropy measures has been published in the articles [1, 4, 16–19, 29]. These articles have shown the applicability and requirements to study the graph entropy measures of different chemical structures. Motivated by the above development, we aim to investigate the various degree and neighborhood degree sum-based entropy measures of the antiviral drug Molnupiravir.

Firstly, we provide the idea of graph entropy measures by employing meaningful information functions according to the standard definitions of degree-based and neighborhood degree sum-based topological indices and do their computational analysis for the drug Molnupiravir. An overview of the two-dimensional structure of Molnupiravir and some basic introductions are provided in Section 2. Next, we have the vertex and edge set partition according to their degree and neighborhood degree. Section 3 consists of the result and discussion: the computation of degree-based and neighborhood degree sum-based entropy measures are presented in Section 3.1 and Section 3.2, respectively. Furthermore, we exhibit the graphical depiction of degree-based entropy and neighborhood degree sum-based entropy measures in respective sections. We compare degree-based and neighborhood degree sum-based topological indices and the corresponding entropy measures of Molnupiravir in Section 4. Finally, we conclude in Section 5.

2 Introduction to Molnupiravir

Late in December 2019, the new coronavirus disease 2019 (COVID-19) was identified as the source of a cluster of pneumonia cases in Wuhan, China. It has immediately spread to various regions of the entire world. Later, COVID-19 was declared a worldwide pandemic by the World Health Organization (WHO) in March 2020 [26]. Patients have the several clinical signs and symptoms of COVID-19 such as fever, sore throat, dry cough, shortness of breath, tiredness, headache, diarrhea, nausea, loss of smell or taste, etc. Concerning COVID-19 infection, there is not a reliable and efficient oral antiviral medication at the moment. Even though, several drugs are being tested on behalf of previous studies to ease the way for a precise treatment for this pandemic. To combat this pandemic, there are some existing drugs such as Theaflavin, Hydroxychloroquine, Remdesivir, Arbidol, Chloroquine, Ritonavir, Lopinavir, Thalidomide, etc. But there is uncertainty that how well these medications work to prevent COVID-19 infection [11].

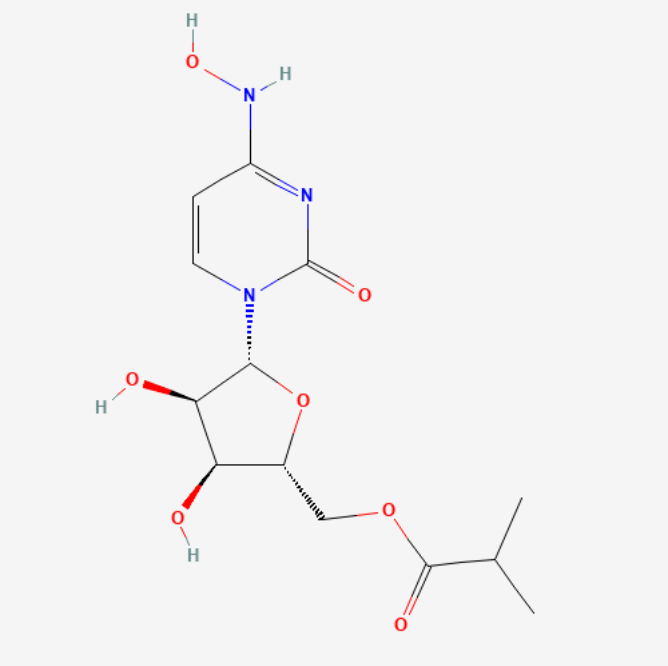


Figure 1: Chemical structure of Molnupiravir ($C_{13}H_{19}N_3O_7$).

A small-molecule oral prodrug having anti-RNA (Ribonucleic Acid) polymerase activity called Molnupiravir, has efficacy against the virus [22]. The drug is also known by the names MK-4482, EIDD-2801, EIDD-1931-isopropyl ester, etc. It causes severe acute respiratory syndrome (SARS-CoV-2) and are currently being studied for the therapy of COVID-19 patients. This oral medication was created at Emory University by Drug Innovation Ventures, and Ridgeback Therapeutics eventually acquired it in collaboration with Merck and Co., USA. All of the above prescription drugs must be provided in a hospital setting, although the fact that some currently have EUAs (emergency use authorizations) for COVID-19. Consequently, since the start of this pandemic, the creation of a basic oral antiviral medication has proven to be an unattainable objective. For more details please refer [5–8, 12, 15]. The two-dimensional chemical structure of Molnupiravir with hydrogen atom is depicted in Figure 1 [25]. The hydrogen-suppressed diagram of the same molecule is displayed in Figure 2 and let us denote it by $\Upsilon = (V(\Upsilon), E(\Upsilon))$.

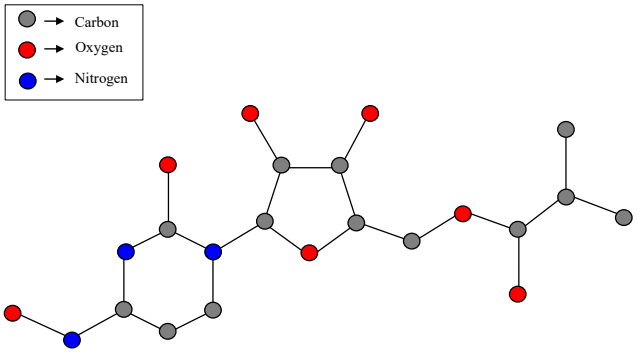


Figure 2: Hydrogen-suppressed diagram of Molnupiravir.

3 Results and Discussions

In this section, we determine degree-based entropy (in Subsection 3.1) and neighborhood degree sum-based entropy measures (in Subsection 3.2) associated with their respective indices for the structure Molnupiravir. For such determination of the entropy measures the values of degree-based topological indices of Υ (Theorem 1) and neighborhood degree-based topological indices of Υ (Theorem 6) are required.

3.1 Degree-Based Entropy Measures of Molnupiravir

Theorem 1 ([8]) *Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be a graph structure of Molnupiravir compound. Then, the degree-based topological indices of Υ are*

(i) $M_1(\Upsilon) = 116$,

(ii) $M_2(\Upsilon) = 136$,

(iii) ${}^{m}M_2(\Upsilon) = \frac{31}{6} \approx 5.1667$,

(iv) $ReZG_3(\Upsilon) = 704$,

(v) $R_\alpha(\Upsilon) = 2^\alpha + 2 \times 3^{\alpha+1} + 2^{2\alpha+1} + 9 \times 6^\alpha + 2 \times 3^{2\alpha+1}$,

(vi) $F(\Upsilon) = 306$,

(vii) $SDD(\Upsilon) = 58$,

(viii) $H(\Upsilon) = \frac{154}{15} \approx 10.2667$,

(ix) $ISI(\Upsilon) = \frac{809}{30} \approx 26.9667$,

(x) $AZI(\Upsilon) = \frac{5907}{32} \approx 184.5938$.

Before proceeding towards the computation of degree-based entropy measures of Molnupiravir, let us have a look at the partition of vertex set (given in Table 1) based on the degrees of the vertices and partition of edge set based on their degrees of the end vertices (given in Table 2).

Table 1: Partition of vertex set of Υ based on the degrees of vertices.

Vertex set	V_1	V_2	V_3
$\boldsymbol{d_\Upsilon(w_1)}$	1	2	3
Total count	7	7	9

Table 2: Partition of edge set of Υ based on the degrees of the end vertices of edges.

Edge set	E_1	E_2	E_3	E_4	E_5
$\boldsymbol{(d_\Upsilon(w_1), d_\Upsilon(w_2))}$	$(1,2)$	$(1,3)$	$(2,2)$	$(2,3)$	$(3,3)$
Total count	1	6	2	9	6

Theorem 2 *Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be a graph structure of Molnupiravir compound. Then, the degree-based entropy measures of Υ are*

(i) $E_{M_1}(\Upsilon) = 3.1623$,

(ii) $E_{M_2}(\Upsilon) = 3.0916$,

(iii) $E_{^mM_2}(\Upsilon) = 3.0724$,

(iv) $E_{ReZG_3}(\Upsilon) = 3.0211$,

(v) $E_{R_\alpha}(\Upsilon) = \log(R_\alpha) - \frac{1}{R_\alpha}\Big[2^\alpha \times \log(2^\alpha) + 6 \times 3^\alpha \times \log(3^\alpha) + 2 \times 2^{2\alpha} \times \log(2^{2\alpha}) + 9 \times 6^\alpha \times \log(6^\alpha) + 6 \times 3^{2\alpha} \times \log(3^{2\alpha})\Big]$,

(vi) $E_F(\Upsilon) = 3.1362$,

(vii) $E_{SDD}(\Upsilon) = 3.1546$,

(viii) $E_H(\Upsilon) = 3.1606$,

(ix) $E_{ISI}(\Upsilon) = 3.1443$,

(x) $E_{AZI}(\Upsilon) = 3.1026$.

Proof: Let us now compute the degree-based entropy measures:

(i) **First Zagreb entropy of *EIDD-2801***

If $\phi(w_1w_2) = d_\Upsilon(w_1) + d_\Upsilon(w_2)$ then using the definition of the First Zagreb index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} d_\Upsilon(w_1) + d_\Upsilon(w_2) = M_1(\Upsilon).$$

From Theorem 1, we have $M_1(\Upsilon) = 116$. Therefore, from Equation (2), the mathematical form of the first Zagreb entropy of a graph Υ is given by

$$E_{M_1}(\Upsilon) = \log(M_1(\Upsilon)) - \frac{1}{M_1(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big).$$

To obtain this entropy, we put the required value from Table 2 in the above equation:

$$\begin{aligned} E_{M_1}(\Upsilon) &= \log(M_1(\Upsilon)) - \frac{1}{M_1(\Upsilon)} \left[\sum_{i=1}^{5} \sum_{w_1w_2 \in E_i(\Upsilon)} \Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big) \right] \\ &= \log(116) - \frac{1}{116} \Big[1 \times (1+2) \times \log(1+2) + 6 \times (1+3) \\ &\quad \times \log(1+3) + 2 \times (2+2) \times \log(2+2) + 9 \times (2+3) \\ &\quad \times \log(2+3) + 6 \times (3+3) \times \log(3+3) \Big] \\ &= \log(116) - \frac{1}{116} \Big[3 \times \log(3) + 24 \times \log(4) + 8 \times \log(4) + 45 \end{aligned}$$

$$\times \log(5) + 36 \times \log(6)\Big]$$
$$= 3.1623,$$

(ii) **Second Zagreb entropy of *EIDD-2801***

If $\phi(w_1w_2) = d_\Upsilon(w_1)d_\Upsilon(w_2)$ then using the definition of the First Zagreb index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} d_\Upsilon(w_1)d_\Upsilon(w_2) = M_2(\Upsilon).$$

From Theorem 1, we get the value $M_2(\Upsilon) = 136$. Now, the given Equation (2) changes to the following mathematical form and is called the Second Zagreb entropy of a graph Υ which is given as

$$E_{M_2}(\Upsilon) = \log(M_2(\Upsilon)) - \frac{1}{M_2(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big).$$

To obtain this entropy we put the necessary value from Table 2 in the above expression:

$$E_{M_2}(\Upsilon) = \log(M_2(\Upsilon)) - \frac{1}{M_2(\Upsilon)} \Bigg[\sum_{i=1}^{5} \sum_{w_1w_2 \in E_i(\Upsilon)} \Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big)\Bigg]$$
$$= \log(136) - \frac{1}{136}\Big[2 \times \log(2) + 18 \times \log(3) + 8 \times \log(4) + 54 \times \log(6) + 54 \times \log(9)\Big]$$
$$= 3.0916,$$

(iii) **Modified second Zagreb entropy of *EIDD-2801***

If $\phi(w_1w_2) = \frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)}$ then using the definition of the modified second Zagreb index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} \frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)} = {}^{m}M_2(\Upsilon).$$

From Theorem 1, we have ${}^{m}M_2(\Upsilon) = \frac{31}{6}$. Therefore, from Equation (2), the mathematical form of the modified second Zagreb entropy of a graph Υ is given by

$$E_{{}^{m}M_2}(\Upsilon) = \log({}^{m}M_2(\Upsilon)) - \frac{1}{{}^{m}M_2(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)} \times \log\left(\frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)}\right).$$

To obtain this entropy we put the required value from Table 2 in the above expression:

$$\begin{aligned} E_{{}^{m}M_2}(\Upsilon) &= \log({}^{m}M_2(\Upsilon)) - \frac{1}{{}^{m}M_2(\Upsilon)} \left[\sum_{i=1}^{5} \sum_{w_1w_2 \in E_i(\Upsilon)} \frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)} \times \log\left(\frac{1}{d_\Upsilon(w_1)d_\Upsilon(w_2)}\right)\right] \\ &= \log\left(\frac{31}{6}\right) - \left(\frac{6}{31}\right)\left[\frac{1}{2} \times \log\left(\frac{1}{2}\right) + 2 \times \log\left(\frac{1}{3}\right) + \frac{1}{2} \times \log\left(\frac{1}{4}\right) + \frac{3}{2} \times \log\left(\frac{1}{6}\right) + \frac{2}{3} \times \log\left(\frac{1}{9}\right)\right] = 3.0724, \end{aligned}$$

(iv) **Redefined third Zagreb entropy of *EIDD-2801***

If $\phi(w_1w_2) = d_\Upsilon(w_1)d_\Upsilon(w_2)(d_\Upsilon(w_1)+d_\Upsilon(w_2))$ then using the definition of the redefined third Zagreb index, we have

$$\begin{aligned} \sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) &= \sum_{w_1w_2 \in E(\Upsilon)} d_\Upsilon(w_1)d_\Upsilon(w_2)(d_\Upsilon(w_1) + d_\Upsilon(w_2)) \\ &= ReZG_3(\Upsilon). \end{aligned}$$

From Theorem 1, we have $ReZG_3(\Upsilon) = 704$. Now, the given Equation (2) changes to the following mathematical form and is called the redefined third Zagreb entropy of a graph Υ.

$$E_{ReZG_3}(\Upsilon) = \log(ReZG_3(\Upsilon)) - \frac{1}{ReZG_3(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} d_\Upsilon(w_1)d_\Upsilon(w_2) \times (d_\Upsilon(w_1) + d_\Upsilon(w_2)).$$

To obtain this entropy we put the necessary value from Table 2 in the above equation:

$$\begin{aligned}
&E_{ReZG_3}(\Upsilon)\\
&= \log(ReZG_3(\Upsilon)) - \frac{1}{ReZG_3(\Upsilon)}\Bigg[\sum_{i=1}^{5}\sum_{w_1w_2\in E_i(\Upsilon)} d_\Upsilon(w_1)\\
&\quad d_\Upsilon(w_2)(d_\Upsilon(w_1)+d_\Upsilon(w_2)) \times \log\Bigg(d_\Upsilon(w_1)d_\Upsilon(w_2)(d_\Upsilon(w_1)+d_\Upsilon(w_2))\Bigg)\Bigg]\\
&= \log(704) - \frac{1}{704}\Big[6\times\log(6) + 72\times\log(12) + 32\times\log(16)\\
&\quad + 270\times\log(30) + 324\times\log(54)\Big] = 3.0211,
\end{aligned}$$

(v) **General Randić entropy of *EIDD-2801***

If $\phi(w_1w_2) = (d_\Upsilon(w_1)d_\Upsilon(w_2))^\alpha$ then using the definition of the general Randić index, we have

$$\sum_{w_1w_2\in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)} (d_\Upsilon(w_1)d_\Upsilon(w_2))^\alpha = R_\alpha(\Upsilon).$$

From Theorem 1, we have $R_\alpha(\Upsilon) = 2^\alpha + 2\times 3^{\alpha+1} + 2^{2\alpha+1} + 9\times 6^\alpha + 2\times 3^{2\alpha+1}$. Now, from Equation (2), the mathematical expression of the general Randić entropy of a graph Υ is given by

$$\begin{aligned}
E_{R_\alpha}(\Upsilon) = \log(R_\alpha(\Upsilon)) - \frac{1}{R_\alpha(\Upsilon)} &\sum_{w_1w_2\in E(\Upsilon)} \Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big)^\alpha\\
&\times \log\Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big)^\alpha.
\end{aligned}$$

To obtain this entropy we put the concerned value from Table 2 in the above equation:

$$\begin{aligned}
E_{R_\alpha}(\Upsilon) = \log(R_\alpha(\Upsilon)) - \frac{1}{R_\alpha(\Upsilon)}&\Bigg[\sum_{i=1}^{5}\sum_{w_1w_2\in E_i(\Upsilon)} \Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big)^\alpha\\
&\times \log\Big(d_\Upsilon(w_1)d_\Upsilon(w_2)\Big)^\alpha\Bigg]
\end{aligned}$$

$$= \log(R_\alpha) - \frac{1}{R_\alpha}\Big[2^\alpha \times \log(2^\alpha) + 6 \times 3^\alpha \times \log(3^\alpha) + 2 \times 2^{2\alpha} \times \log(2^{2\alpha}) + 9 \times 6^\alpha \times \log(6^\alpha) + 6 \times 3^{2\alpha} \times \log(3^{2\alpha})\Big],$$

(vi) **Forgotten entropy of *EIDD-2801***

If $\phi(w_1w_2) = (d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2$ then using the definition of the Forgotten index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} (d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2 = F(\Upsilon).$$

From Theorem 1, we have $F(\Upsilon) = 306$. Now, from Equation (2), the mathematical form of the forgotten entropy of a graph Υ which is given as

$$E_F(\Upsilon) = \log(F(\Upsilon)) - \frac{1}{F(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \Big((d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2\Big) \times \log\Big((d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2\Big).$$

To obtain this entropy we put the required value from Table 2 in the above equation:

$$E_F(\Upsilon) = \log(F(\Upsilon)) - \frac{1}{F(\Upsilon)}\left[\sum_{i=1}^{5} \sum_{w_1w_2 \in E_i(\Upsilon)} \Big((d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2\Big) \times \log\Big((d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2\Big)\right]$$

$$= \log(306) - \frac{1}{306}\Big[5 \times \log(5) + 60 \times \log(10) + 16 \times \log(8) + 117 \times \log(13) + 108 \times \log(18)\Big] = 3.1362,$$

(vii) **Symmetric division (deg) entropy of *EIDD-2801***

If $\phi(w_1w_2) = \frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1)d_\Upsilon(w_2)}$ then using the definition of the symmetric division (deg) index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} \frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1)d_\Upsilon(w_2)} = SDD(\Upsilon).$$

From Theorem 1, we have $SDD(\Upsilon) = 58$. Therefore, from Equation (2), the mathematical form of the symmetric division (deg) entropy of a graph Υ is given as

$$\begin{aligned}
&E_{SDD}(\Upsilon)\\
&= \log(SDD(\Upsilon)) - \frac{1}{SDD(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \left(\frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1) d_\Upsilon(w_2)} \right)\\
&\quad \times \log \left(\frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1) d_\Upsilon(w_2)} \right).
\end{aligned}$$

To obtain this entropy we put the necessary value from Table 2 in the above expression:

$$\begin{aligned}
&E_{SDD}(\Upsilon)\\
&= \log(SDD(\Upsilon)) - \frac{1}{SDD(\Upsilon)} \left[\sum_{i=1}^{5} \sum_{w_1w_2 \in E_i(\Upsilon)} \left(\frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1) d_\Upsilon(w_2)} \right) \right.\\
&\quad \left. \times \log \left(\frac{(d_\Upsilon(w_1))^2 + (d_\Upsilon(w_2))^2}{d_\Upsilon(w_1) d_\Upsilon(w_2)} \right) \right]\\
&= \log(58) - \frac{1}{58} \left[\frac{5}{2} \times \log \left(\frac{5}{2} \right) + 20 \times \log \left(\frac{10}{3} \right) + 4 \times \log(2) + \frac{39}{2} \right.\\
&\quad \left. \times \log \left(\frac{13}{6} \right) + 12 \times \log(2) \right] = 3.1546,
\end{aligned}$$

(viii) **Harmonic entropy of *EIDD-2801***

If $\phi(w_1w_2) = \frac{2}{d_\Upsilon(w_1) + d_\Upsilon(w_2)}$ then using the definition of the Harmonic index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \phi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} \frac{2}{d_\Upsilon(w_1) + d_\Upsilon(w_2)} = H(\Upsilon).$$

From Theorem 1, we have $H(\Upsilon) = \frac{154}{15}$. Now, from Equation (2), the mathematical expression of the Harmonic entropy of a graph Υ is given by

$$E_H(\Upsilon) = \log(H(\Upsilon)) - \frac{1}{H(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \left(\frac{2}{d_\Upsilon(w_1) + d_\Upsilon(w_2)} \right)$$

$$\times \log\left(\frac{2}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right).$$

To obtain this entropy we put the necessary value from Table 2 in the following manner:

$$\begin{aligned} E_H(\Upsilon) &= \log(H(\Upsilon)) - \frac{1}{H(\Upsilon)}\left[\sum_{i=1}^{5}\sum_{w_1w_2\in E_i(\Upsilon)}\left(\frac{2}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right)\right. \\ &\quad \left.\times \log\left(\frac{2}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right)\right] \\ &= \log\left(\frac{154}{15}\right) - \frac{15}{154}\left[\frac{2}{3}\times\log\left(\frac{2}{3}\right)+3\times\log\left(\frac{1}{2}\right)+1\right. \\ &\quad \left.\times\log\left(\frac{1}{2}\right)+\frac{18}{5}\times\log\left(\frac{2}{5}\right)+2\times\log\left(\frac{1}{3}\right)\right] = 3.1606, \end{aligned}$$

(ix) **Inverse sum (indeg) entropy of *EIDD-2801***

If $\phi(w_1w_2) = \frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}$ then using the definition of the Inverse sum (indeg) index, we have

$$\sum_{w_1w_2\in E(\Upsilon)}\phi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)}\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)} = ISI(\Upsilon).$$

From Theorem 1, we have $ISI(\Upsilon) = \frac{809}{30}$. Therefore, from Equation (2), the mathematical expression of the inverse sum (indeg) entropy of a graph Υ is given by

$$\begin{aligned} E_{ISI}(\Upsilon) &= \log(ISI(\Upsilon)) - \frac{1}{ISI(\Upsilon)}\sum_{w_1w_2\in E(\Upsilon)}\left(\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right) \\ &\quad \times\log\left(\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right). \end{aligned}$$

To obtain this entropy we put the concerned value from Table 2 in the above equation:

$$E_{ISI}(\Upsilon) = \log(ISI(\Upsilon)) - \frac{1}{ISI(\Upsilon)}\left[\sum_{i=1}^{5}\sum_{w_1w_2\in E_i(\Upsilon)}\left(\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right)\right.$$

$$\times \log\left(\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)}\right)\Bigg]$$
$$= \log\left(\frac{809}{30}\right) - \frac{30}{809}\left[\frac{2}{3}\times\log\left(\frac{2}{3}\right)+\frac{9}{2}\times\log\left(\frac{3}{4}\right)+2\times\log(1)\right.$$
$$\left.+\frac{54}{5}\times\log\left(\frac{6}{5}\right)+9\times\log\left(\frac{3}{2}\right)\right] = 3.1443,$$

(x) **Augmented Zagreb entropy of *EIDD-2801***

If $\phi(w_1w_2) = \left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3$ then using the definition of the Augmented Zagreb index, we have

$$\sum_{w_1w_2\in E(\Upsilon)}\phi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)}\left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3 = AZI(\Upsilon).$$

From Theorem 1, we have $AZI(\Upsilon) = \frac{5907}{32} \approx 184.5938$. Therefore, from Equation (2), the mathematical form of the augmented Zagreb entropy of a graph Υ is given as

$$E_{AZI}(\Upsilon) = \log(AZI(\Upsilon)) - \frac{1}{AZI(\Upsilon)}\sum_{w_1w_2\in E(\Upsilon)}\left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3$$
$$\times\log\left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3.$$

To obtain this entropy we put the required value from Table 2 in the above expression:

$$E_{AZI}(\Upsilon)$$
$$= \log(AZI(\Upsilon)) - \frac{1}{AZI(\Upsilon)}\left[\sum_{i=1}^{5}\sum_{w_1w_2\in E_i(\Upsilon)}\left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3\right.$$
$$\left.\times\log\left\{\frac{d_\Upsilon(w_1)d_\Upsilon(w_2)}{d_\Upsilon(w_1)+d_\Upsilon(w_2)-2}\right\}^3\right]$$
$$= \log\left(\frac{5907}{32}\right) - \frac{32}{5907}\left[8\times\log(8)+\frac{81}{4}\times\log\left(\frac{27}{8}\right)+16\times\log(8)\right.$$
$$\left.+72\times\log(8)+\frac{2187}{32}\times\log\left(\frac{729}{64}\right)\right] = 3.1026.$$

□

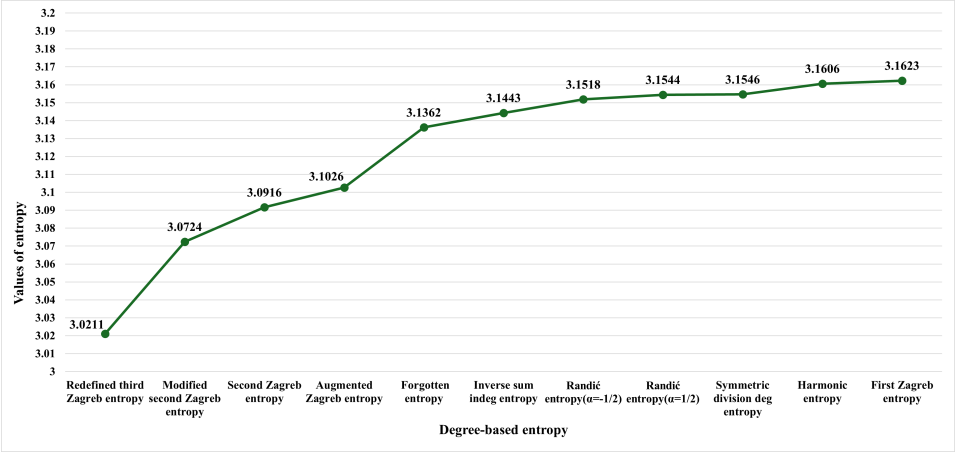


Figure 3: Visual depiction of degree-based entropy measures for Molnupiravir.

Further, Figure 3 exhibits the graphical representation of degree-based entropy measures for the COVID-19 drug Molnupiravir. These entropies are neatly placed in ascending order in the figure, showing that the degree-based entropies and their related values are plotted on the x and y axes, respectively.

Remark 3 *It is noticeable from the Figure 3 that the redefined third Zagreb entropy* (E_{ReZG_3}) *acquires the lowest value as 3.0211, while the first Zagreb entropy* (E_{M_1}) *gets the highest value as 3.1623.*

Remark 4 *For the drug Molnupiravir* Υ*, we observe:*

- *from Theorem 1 that the degree-based topological indices maintain the following relationship:*

  $$^{m}M_2 < H < R_{-1/2} < ISI < R_{1/2} < SDD < M_1 < M_2 < AZI < F < ReZG_3$$

  and

- *from Figure 3 that the corresponding entropies maintain the following relationship:*

  $$E_{ReZG_3} < E_{^{m}M_2} < E_{M_2} < E_{AZI} < E_F < E_{ISI} < E_{R_{-1/2}} < E_{R_{1/2}} < E_{SDD} < E_H < E_{M_1}.$$

3.2 Neighborhood Degree Sum-Based Entropy Measures of Molnupiravir

Theorem 5 ([7]) *Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be a graph structure of Molnupiravir compound. Then, the neighborhood degree sum-based topological indices of Υ are*

(i) $NM_1(\Upsilon) = 272$,

(ii) $NM_2(\Upsilon) = 783$,

(iii) ${}^{nm}M_2(\Upsilon) = \frac{219971}{235200} \approx 0.9353$,

(iv) $ND_3(\Upsilon) = 9692$,

(v) $NR_\alpha(\Upsilon) = 2^{3\alpha}+2\times 15^\alpha+2^{\alpha+1}\times 3^{2\alpha}+2\times 21^\alpha+2^{3\alpha}\times 3^\alpha+2\times 5^{2\alpha}+3^{\alpha+1}\times 10^\alpha+35^\alpha+2^{3\alpha}\times 5^\alpha+2^{2\alpha+1}\times 3^{2\alpha}+42^\alpha+2^{4\alpha+1}\times 3^\alpha+2\times 7^{2\alpha}+56^\alpha+2^{6\alpha}$,

(vi) $NF(\Upsilon) = 1658$,

(vii) $ND_5(\Upsilon) = \frac{1833}{35} \approx 52.3714$,

(viii) $NH(\Upsilon) = \frac{1607453}{360360} \approx 4.4607$,

(ix) $NI(\Upsilon) = \frac{197237}{3003} \approx 65.6799$,

(x) $S(\Upsilon) = \frac{428161963287795409}{433297296432000} \approx 988.1483$.

In this section, we first look into the partition of the vertex set (given in Table 3) of the graph based on the neighborhood degrees of the vertices, and the edge set partition (as shown in Table 4) based on the neighborhood degrees of end vertices of the edges.

Table 3: Partition of vertex set of Υ based on the neighborhood degrees of end vertices.

Vertex set	V_1	V_2	V_3	V_4	V_5	V_6	V_7
$\tau(w_1)$	2	3	4	5	6	7	8
Total count	1	6	1	5	5	3	2

Theorem 6 ([7]) *Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be a graph structure of Molnupiravir compound. Then, the neighborhood degree sum-based entropy measures of Υ are*

Table 4: Partition of edge set of Υ based on their neighborhood degrees of end vertices of edges.

Edge set	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
$(\tau(w_1), \tau(w_2))$	$(2,4)$	$(3,5)$	$(3,6)$	$(3,7)$	$(4,6)$	$(5,5)$	$(5,6)$	$(5,7)$
Total count	1	2	2	2	1	2	3	1

Edge set	E_9	E_{10}	E_{11}	E_{12}	E_{13}	E_{14}	E_{15}
$(\tau(w_1), \tau(w_2))$	$(6,7)$	$(6,8)$	$(7,7)$	$(7,8)$	$(8,8)$	$(5,8)$	$(6,6)$
Total count	1	2	2	1	1	1	2

(i) $E_{NM_1}(\Upsilon) = 3.1545$,

(ii) $E_{NM_2}(\Upsilon) = 3.0811$,

(iii) $E_{^{nm}M_2}(\Upsilon) = 3.0350$,

(iv) $E_{ND_3}(\Upsilon) = 2.9901$,

(v) $E_{NR_\alpha}(\Upsilon) = \log(NR_\alpha) - \frac{1}{NR_\alpha}\Big[8^\alpha \log(8^\alpha) + 2 \times 15^\alpha \log(15^\alpha) + 2 \times 18^\alpha \log(18^\alpha) + 2 \times 21^\alpha \log(21^\alpha) + 24^\alpha \log(24^\alpha) + 2 \times 25^\alpha \log(25^\alpha) + 3 \times 30^\alpha \log(30^\alpha) + 35^\alpha \log(35^\alpha) + 40^\alpha \log(40^\alpha) + 2 \times 36^\alpha \log(36^\alpha) + 42^\alpha \log(42^\alpha) + 2 \times 48^\alpha \log(48^\alpha) + 2 \times 49^\alpha \log(49^\alpha) + 56^\alpha \log(56^\alpha) + 64^\alpha \log(64^\alpha)\Big]$,

(vi) $E_{NF}(\Upsilon) = 3.1017$,

(vii) $E_{ND_5}(\Upsilon) = 3.4990$,

(viii) $E_{NH}(\Upsilon) = 3.1496$,

(ix) $E_{NI}(\Upsilon) = 3.1470$,

(x) $E_S(\Upsilon) = 4.6389$.

Proof: We then move to evaluate the neighborhood degree sum-based entropy measures of the drug Molnupiravir.

(i) **Neighborhood first Zagreb entropy of *EIDD-2801***

If $\psi(w_1w_2) = \tau(w_1) + \tau(w_2)$ then using the definition of the neighborhood first Zagreb index, we have

$$\sum_{w_1w_2 \in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} \tau(w_1) + \tau(w_2) = NM_1(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{NM_1}(\Upsilon) = \log(NM_1(\Upsilon)) - \frac{1}{NM_1(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \Big(\tau(w_1) + \tau(w_2)\Big) \times \log\Big(\tau(w_1) + \tau(w_2)\Big).$$

To obtain this entropy we put the value of $NM_1(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$\begin{aligned}
E_{NM_1}(\Upsilon) &= \log(NM_1(\Upsilon)) - \frac{1}{NM_1(\Upsilon)} \left[\sum_{i=1}^{15} \sum_{w_1w_2 \in E_i(\Upsilon)} \Big(\tau(w_1) + \tau(w_2)\Big) \times \log\Big(\tau(w_1) + \tau(w_2)\Big) \right] \\
&= \log(272) - \frac{1}{272} \Big[1 \times (2+4)\log(2+4) + 2 \times (3+5) \\
&\quad \log(3+5) + 2 \times (3+6)\log(3+6) + 2 \times (3+7)\log(3+7) \\
&\quad + 1 \times (4+6)\log(4+6) + 2 \times (5+5)\log(5+5) + 3 \times (5 \\
&\quad + 6)\log(5+6) + 1 \times (5+7)\log(5+7) + 1 \times (5+8) \\
&\quad \log(5+8) + 2 \times (6+6)\log(6+6) + 1 \times (6+7)\log(6+7) \\
&\quad + 2 \times (6+8)\log(6+8) + 2 \times (7+7)\log(7+7) + 1 \times (7 \\
&\quad + 8)\log(7+8) + 1 \times (8+8)\log(8+8) \Big] \\
&= \log(272) - \frac{1}{272} \Big[6\log(6) + 16\log(8) + 18\log(9) + 20 \\
&\quad \times \log(10) + 10\log(10) + 20\log(10) + 33\log(11) + 12 \\
&\quad \times \log(12) + 13\log(13) + 24\log(12) + 13\log(13) + 28 \\
&\quad \times \log(14) + 28\log(14) + 15\log(15) + 16\log(16) \Big] \\
&= 3.1545,
\end{aligned}$$

(ii) **Neighborhood second Zagreb entropy of *EIDD-2801***

If $\psi(w_1w_2) = \tau(w_1)\tau(w_2)$, then

$$\sum_{w_1w_2\in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)} \tau(w_1)\tau(w_2) = NM_2(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{NM_2}(\Upsilon) = \log(NM_2(\Upsilon)) - \frac{1}{NM_2(\Upsilon)} \sum_{w_1w_2\in E(\Upsilon)} \Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big).$$

To obtain this entropy we put the required value of $NM_2(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$\begin{aligned}
&E_{NM_2}(\Upsilon)\\
&= \log(NM_2(\Upsilon)) - \frac{1}{NM_2(\Upsilon)}\left[\sum_{i=1}^{15} \sum_{w_1w_2\in E_i(\Upsilon)} \Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big) \times \log\Big(d_\Upsilon(w_1) + d_\Upsilon(w_2)\Big)\right]\\
&= \log(783) - \frac{1}{783}\Big[8\log(8) + 30\log(15) + 36\log(18) + 42\log(21)\\
&\quad + 24\log(24) + 50\log(25) + 90\log(30) + 35\log(35) + 40\log(40)\\
&\quad + 72\log(36) + 42\log(42) + 96\log(48) + 98\log(49) + 56\log(56)\\
&\quad + 64\log(64)\Big] = 3.0811,
\end{aligned}$$

(iii) **Neighborhood modified second Zagreb entropy of *EIDD-2801***

If $\psi(w_1w_2) = \frac{1}{\tau(w_1)\tau(w_2)}$, then

$$\sum_{w_1w_2\in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)} \frac{1}{\tau(w_1)\tau(w_2)} = {}^{nm}M_2(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{^{nm}M_2}(\Upsilon) = \log(^{nm}M_2(\Upsilon)) - \frac{1}{^{nm}M_2(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \frac{1}{\tau(w_1)\tau(w_2)} \times \log\left(\frac{1}{\tau(w_1)\tau(w_2)}\right).$$

To obtain this entropy we put the value of $^{nm}M_2(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$\begin{aligned}
&E_{^{nm}M_2}(\Upsilon)\\
&= \log(^{nm}M_2(\Upsilon)) - \frac{1}{^{nm}M_2(\Upsilon)}\left[\sum_{i=1}^{15} \sum_{w_1w_2 \in E_i(\Upsilon)} \frac{1}{\tau(w_1)\tau(w_2)} \times \log\left(\frac{1}{\tau(w_1)\tau(w_2)}\right)\right]\\
&= \log\left(\frac{219971}{235200}\right) - \left(\frac{235200}{219971}\right)\left[\frac{1}{8}\log\left(\frac{1}{8}\right) + \frac{2}{15}\log\left(\frac{1}{15}\right) + \frac{2}{18} \times \log\left(\frac{1}{18}\right) + \frac{2}{21}\log\left(\frac{1}{21}\right) + \frac{1}{24}\log\left(\frac{1}{24}\right) + \frac{2}{25}\log\left(\frac{1}{25}\right) + \frac{1}{10} \times \log\left(\frac{1}{30}\right) + \frac{1}{35}\log\left(\frac{1}{35}\right) + \frac{1}{40}\log\left(\frac{1}{40}\right) + \frac{1}{18}\log\left(\frac{1}{36}\right) + \frac{1}{42} \times \log\left(\frac{1}{42}\right) + \frac{1}{24}\log\left(\frac{1}{48}\right) + \frac{2}{49}\log\left(\frac{1}{49}\right) + \frac{1}{56}\log\left(\frac{1}{56}\right) + \frac{1}{64} \times \log\left(\frac{1}{64}\right)\right] = 3.0350,
\end{aligned}$$

(iv) **Third ND_e entropy of *EIDD-2801***

If $\psi(w_1w_2) = \tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2))$, then

$$\sum_{w_1w_2 \in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} \tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2)) = ND_3.$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is

given by

$$E_{ND_3}(\Upsilon) = \log(ND_3(\Upsilon)) - \frac{1}{ND_3(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2)) \times \log\Big(\tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2))\Big)$$

To obtain this entropy we put the value of $ND_3(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$\begin{aligned}
&E_{ND_3}(\Upsilon)\\
&= \log(ND_3(\Upsilon)) - \frac{1}{ND_3(\Upsilon)}\Bigg[\sum_{i=1}^{15} \sum_{w_1w_2 \in E_i(\Upsilon)} \tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2))\\
&\quad \times \log\Big(\tau(w_1)\tau(w_2)(\tau(w_1) + \tau(w_2))\Big)\Bigg]\\
&= \log(9692) - \frac{1}{9692}\Big[48\log(48) + 240\log(120) + 324\log(162) + 420\\
&\quad \times \log(210) + 240\log(240) + 500\log(250) + 990\log(330) + 420\\
&\quad \times \log(420) + 520\log(520) + 864\log(432) + 546\log(546) + 1344\\
&\quad \times \log(672) + 1372\log(686) + 840\log(840) + 1024\log(1024)\Big]\\
&= 2.9901,
\end{aligned}$$

(v) **Neighborhood general Randić entropy of *EIDD-2801***

If $\psi(w_1w_2) = (\tau(w_1)\tau(w_2))^{\alpha}$, then

$$\sum_{w_1w_2 \in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2 \in E(\Upsilon)} (\tau(w_1)\tau(w_2))^{\alpha} = NR_{\alpha}(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{NR_{\alpha}}(\Upsilon) = \log(NR_{\alpha}(\Upsilon)) - \frac{1}{NR_{\alpha}(\Upsilon)} \sum_{w_1w_2 \in E(\Upsilon)} \Big(\tau(w_1)\tau(w_2)\Big)^{\alpha} \times \log\Big(\tau(w_1)\tau(w_2)\Big)^{\alpha}.$$

To obtain this entropy we put the value of $NR_\alpha(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$
\begin{aligned}
&E_{NR_\alpha}(\Upsilon)\\
&= \log(NR_\alpha(\Upsilon)) - \frac{1}{NR_\alpha(\Upsilon)}\left[\sum_{i=1}^{15}\sum_{w_1w_2\in E_i(\Upsilon)}\Big(\tau(w_1)\tau(w_2)\Big)^\alpha\right.\\
&\quad\left.\times\log\Big(\tau(w_1)\tau(w_2)\Big)^\alpha\right]\\
&= \log\left(NR_\alpha\right) - \frac{1}{NR_\alpha}\Big[8^\alpha\log(8^\alpha) + 2\times15^\alpha\log(15^\alpha) + 2\times18^\alpha\log(18^\alpha)\\
&\quad + 2\times21^\alpha\log(21^\alpha) + 24^\alpha\log(24^\alpha) + 2\times25^\alpha\log(25^\alpha) + 3\times30^\alpha\\
&\quad\times\log(30^\alpha) + 35^\alpha\log(35^\alpha) + 40^\alpha\log(40^\alpha) + 2\times36^\alpha\log(36^\alpha) + 42^\alpha\\
&\quad\times\log(42^\alpha) + 2\times48^\alpha\log(48^\alpha) + 2\times49^\alpha\log(49^\alpha) + 56^\alpha\log(56^\alpha)\\
&\quad + 64^\alpha\log(64^\alpha)\Big],
\end{aligned}
$$

(vi) **Neighborhood forgotten entropy of *EIDD-2801***

If $\psi(w_1w_2) = (\tau(w_1))^2 + (\tau(w_2))^2$, then

$$\sum_{w_1w_2\in E(\Upsilon)}\psi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)}(\tau(w_1))^2 + (\tau(w_2))^2 = NF(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$
\begin{aligned}
E_{NF}(\Upsilon) = \log(NF(\Upsilon)) &- \frac{1}{NF(\Upsilon)}\sum_{w_1w_2\in E(\Upsilon)}\Big((\tau(w_1))^2 + (\tau(w_2))^2\Big)\\
&\times\log\Big((\tau(w_1))^2 + (\tau(w_2))^2\Big).
\end{aligned}
$$

To obtain this entropy we put the value of $NF(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$
\begin{aligned}
&E_{NF}(\Upsilon)\\
&= \log(NF(\Upsilon)) - \frac{1}{NF(\Upsilon)}\left[\sum_{i=1}^{15}\sum_{w_1w_2\in E_i(\Upsilon)}\Big((\tau(w_1))^2 + (\tau(w_2))^2\Big)\right.
\end{aligned}
$$

$$\times \log\left((\tau(w_1))^2 + (\tau(w_2))^2\right)\Bigg]$$

$$= \log(1658) - \frac{1}{1658}\Big[20\log(20) + 68\log(34) + 90\log(45) + 116\log(58) + 52\log(52) + 100\log(50) + 183\log(61) + 74\log(74) + 89\log(89) + 144\log(72) + 85\log(85) + 200\log(100) + 196\log(98) + 113 \times \log(113) + 128\log(128)\Big] = 3.1017,$$

(vii) **Fifth $\mathbf{ND_e}$ entropy of *EIDD-2801***

If $\psi(w_1w_2) = \frac{(\tau(w_1))^2+(\tau(w_2))^2}{\tau(w_1)\tau(w_2)}$, then

$$\sum_{w_1w_2\in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)} \frac{(\tau(w_1))^2 + (\tau(w_2))^2}{\tau(w_1)\tau(w_2)} = ND_5(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{ND_5}(\Upsilon) = \log(ND_5(\Upsilon)) - \frac{1}{ND_5(\Upsilon)} \sum_{w_1w_2\in E(\Upsilon)} \left(\frac{(\tau(w_1))^2 + (\tau(w_2))^2}{\tau(w_1)\tau(w_2)}\right) \times \log\left(\frac{(\tau(w_1))^2 + (\tau(w_2))^2}{\tau(w_1)\tau(w_2)}\right).$$

To obtain this entropy we put the value of $ND(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$E_{ND_5}(\Upsilon)$$

$$= \log(ND_5(\Upsilon)) - \frac{1}{ND_5(\Upsilon)}\left[\sum_{i=1}^{15} \sum_{w_1w_2\in E_i(\Upsilon)} \left(\frac{(\tau(w_1))^2 + (\tau(w_2))^2}{\tau(w_1)\tau(w_2)}\right) \times \log\left(\frac{(\tau(w_1))^2 + (\tau(w_2))^2}{\tau(w_1)\tau(w_2)}\right)\right]$$

$$= \log\left(\frac{1833}{35}\right) - \frac{35}{1833}\left[\left(\frac{20}{8}\right)\log\left(\frac{20}{8}\right) + \left(\frac{68}{15}\right)\log\left(\frac{34}{15}\right)\right.$$

$$+\left(\frac{90}{18}\right)\log\left(\frac{45}{18}\right)+\left(\frac{116}{21}\right)\log\left(\frac{58}{21}\right)+\left(\frac{52}{24}\right)\log\left(\frac{52}{24}\right)+4\log(2)$$
$$+\left(\frac{183}{30}\right)\log\left(\frac{61}{30}\right)+\left(\frac{74}{35}\right)\log\left(\frac{74}{35}\right)+\left(\frac{89}{40}\right)\log\left(\frac{89}{40}\right)$$
$$+\left(\frac{144}{36}\right)\log\left(\frac{72}{36}\right)+\left(\frac{85}{42}\right)\log\left(\frac{85}{42}\right)+\left(\frac{200}{48}\right)\log\left(\frac{100}{48}\right)$$
$$+\left(\frac{196}{49}\right)\log\left(\frac{98}{49}\right)+\left(\frac{113}{56}\right)\log\left(\frac{113}{56}\right)+\left(\frac{128}{64}\right)\log(2)\Bigg]$$
$$=3.4990,$$

(viii) **Neighborhood Harmonic entropy of *EIDD-2801***

If $\psi(w_1w_2)=\frac{2}{\tau(w_1)+\tau(w_2)}$, then

$$\sum_{w_1w_2\in E(\Upsilon)}\psi(w_1w_2)=\sum_{w_1w_2\in E(\Upsilon)}\frac{2}{\tau(w_1)+\tau(w_2)}=NH(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood first Zagreb entropy of a graph Υ which is given by

$$E_{NH}(\Upsilon)=\log(NH(\Upsilon))-\frac{1}{NH(\Upsilon)}\sum_{w_1w_2\in E(\Upsilon)}\left(\frac{2}{\tau(w_1)+\tau(w_2)}\right)\times\log\left(\frac{2}{\tau(w_1)+\tau(w_2)}\right).$$

To obtain this entropy we put the value of $NH(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$E_{NH}(\Upsilon)$$
$$=\log(NH(\Upsilon))-\frac{1}{NH(\Upsilon)}\Bigg[\sum_{i=1}^{15}\sum_{w_1w_2\in E_i(\Upsilon)}\left(\frac{2}{\tau(w_1)+\tau(w_2)}\right)\times\log\left(\frac{2}{\tau(w_1)+\tau(w_2)}\right)\Bigg]$$
$$=\log\left(\frac{1607453}{360360}\right)-\frac{360360}{1607453}\Bigg[\frac{1}{3}\log\left(\frac{1}{3}\right)+\frac{1}{2}\log\left(\frac{1}{4}\right)+\frac{4}{9}\log\left(\frac{2}{9}\right)$$

$$+\frac{2}{5}\log\left(\frac{1}{5}\right)+\frac{1}{5}\log\left(\frac{1}{5}\right)+\frac{2}{5}\log\left(\frac{1}{5}\right)+\frac{6}{11}\log\left(\frac{2}{11}\right)+\frac{1}{6}\log\left(\frac{1}{6}\right)$$
$$+\frac{2}{13}\log\left(\frac{2}{13}\right)+\frac{1}{3}\log\left(\frac{1}{6}\right)+\frac{2}{13}\log\left(\frac{2}{13}\right)+\frac{2}{7}\log\left(\frac{1}{7}\right)+\frac{2}{7}$$
$$\times\log\left(\frac{1}{7}\right)+\frac{2}{15}\log\left(\frac{2}{15}\right)+\frac{1}{8}\log\left(\frac{1}{8}\right)\Bigg]=3.1496,$$

(ix) **Neighborhood Inverse sum entropy of *EIDD-2801***

If $\psi(w_1w_2)=\frac{\tau(w_1)d_\Upsilon(w_2)}{\tau(w_1)+\tau(w_2)}$, then

$$\sum_{w_1w_2\in E(\Upsilon)}\psi(w_1w_2)=\sum_{w_1w_2\in E(\Upsilon)}\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)}=NI(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the neighborhood Inverse sum entropy of a graph Υ which is given by

$$E_{NI}(\Upsilon)=\log(NI(\Upsilon))-\frac{1}{NI(\Upsilon)}\sum_{w_1w_2\in E(\Upsilon)}\left(\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)}\right)$$
$$\times\log\left(\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)}\right).$$

To obtain this entropy we put the value of $NI(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$E_{NI}(\Upsilon)$$
$$=\log(NI(\Upsilon))-\frac{1}{NI(\Upsilon)}\Bigg[\sum_{i=1}^{15}\sum_{w_1w_2\in E_i(\Upsilon)}\left(\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)}\right)$$
$$\times\log\left(\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)}\right)\Bigg]$$
$$=\log\left(\frac{197237}{3003}\right)-\frac{3003}{197237}\Bigg[\frac{4}{3}\log\left(\frac{4}{3}\right)+\frac{15}{4}\log\left(\frac{15}{8}\right)+4\log(2)$$
$$+\frac{21}{5}\log\left(\frac{21}{10}\right)+\frac{12}{5}\log\left(\frac{12}{5}\right)+5\log\left(\frac{5}{2}\right)+\frac{90}{11}\log\left(\frac{30}{11}\right)+\frac{35}{12}$$

$$\times \log\left(\frac{35}{12}\right) + \frac{40}{13}\log\left(\frac{40}{13}\right) + 6\log(3) + \frac{42}{13}\log\left(\frac{42}{13}\right) + \frac{48}{7}$$
$$\times \log\left(\frac{24}{7}\right) + 7\log\left(\frac{7}{2}\right) + \frac{56}{15}\log\left(\frac{56}{15}\right) + 4\log(4)\Bigg] = 3.1470,$$

(x) **Sanskruti entropy of *EIDD-2801***

If $\psi(w_1w_2) = \left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3$, then

$$\sum_{w_1w_2\in E(\Upsilon)} \psi(w_1w_2) = \sum_{w_1w_2\in E(\Upsilon)} \left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3 = S(\Upsilon).$$

Now, the obtained Equation 2 reduced to the following expression and is called the Sanskruti entropy of a graph Υ which is given by

$$E_S(\Upsilon) = \log(S(\Upsilon)) - \frac{1}{S(\Upsilon)} \sum_{w_1w_2\in E(\Upsilon)} \left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3$$
$$\times \log\left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3.$$

To obtain this entropy we put the value of $S(\Upsilon)$ from Theorem 6 and using Table 4, in the following manner:

$$E_S(\Upsilon)$$
$$= \log(S(\Upsilon)) - \frac{1}{S(\Upsilon)}\left[\sum_{i=1}^{15} \sum_{w_1w_2\in E_i(\Upsilon)} \left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3\right.$$
$$\left.\times \log\left\{\frac{\tau(w_1)\tau(w_2)}{\tau(w_1)+\tau(w_2)-2}\right\}^3\right]$$
$$= \log\left(\frac{428161963287795409}{433297296432000}\right) - \frac{433297296432000}{428161963287795409}\Bigg[8\log(8)$$
$$+ \frac{125}{4}\log\left(\frac{125}{8}\right) + \frac{11664}{343}\log\left(\frac{5832}{343}\right) + \frac{9261}{256}\log\left(\frac{9261}{512}\right) + 27$$
$$\times \log(27) + \frac{15625}{256}\log\left(\frac{15625}{512}\right) + \frac{1000}{9}\log\left(\frac{1000}{27}\right) + \frac{343}{8}$$
$$\times \log\left(\frac{343}{8}\right) + \frac{64000}{1331}\log\left(\frac{64000}{1331}\right) + \frac{11664}{125}\log\left(\frac{5832}{125}\right) + \frac{74088}{1331}$$

$$\times \log\left(\frac{74088}{1331}\right) + 128\log(64) + \frac{117649}{864}\log\left(\frac{117649}{1728}\right) + \frac{175616}{2197} \times \log\left(\frac{175616}{2197}\right) + \frac{32768}{343}\log\left(\frac{32768}{343}\right)\Bigg] = 4.6389.$$

□

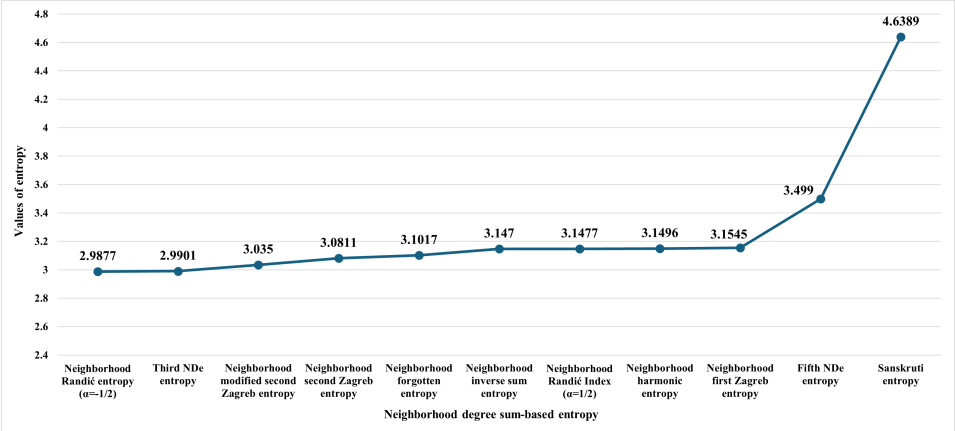


Figure 4: Visual depiction of neighborhood degree sum-based entropy measures for Molnupiravir.

The graphical demonstration of the considered neighborhood degree sum-based entropy measures for the drug Molnupiravir are exhibited in Figure 4. The figure neatly places these entropies in ascending order, showing that the neighborhood degree sum-based entropies and their associated values are plotted on the x and y axes, respectively.

Remark 7 *Figure 4 signifies that the neighborhood Randić entropy ($\alpha = -1/2$) reports the minimum value of 2.9877 and the Sanskruti entropy takes the maximum value of 4.6389.*

Remark 8 *For the drug Molnupiravir Υ, we observe*

- *from Theorem 6 that the neighborhood degree sum-based topological indices maintain the following relationship:*

  $${}^{nm}M_2 < NH < NR_{-1/2} < ND_5 < NI < NR_{1/2} < NM_1 < NM_2 < S < NF < ND_3$$

  and

- *from Figure 4 that the neighborhood degree sum-based entropies maintain the following relationship:*

$$E_{NR_{-1/2}} < E_{ND_3} < E_{^{nm}M_2} < E_{NM_2} < E_{NF} < E_{NI} < E_{NR_{1/2}} < E_{NH} < E_{NM_1} < E_{ND_5} < E_S.$$

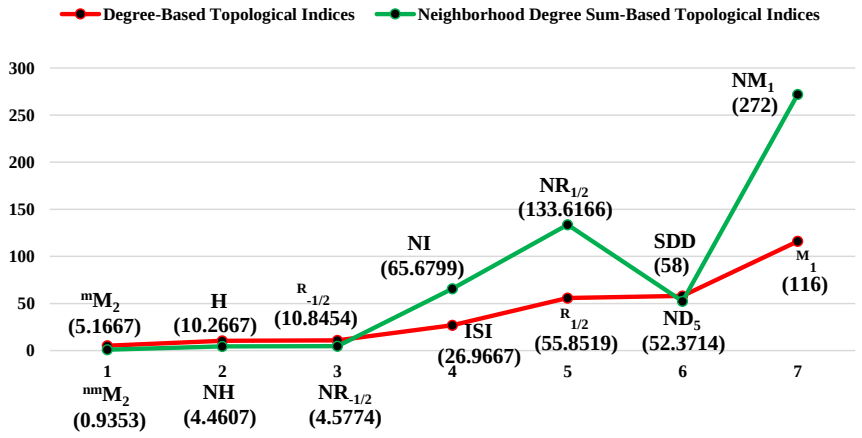
4 Comparative Evaluation Between the Topological Indices and Entropy Measures of Molnupiravir

This section presents a comparative study between degree-based and neighborhood degree sum-based topological indices and their associated entropy measures of Molnupiravir. The numerical values of each of the classes of topological indices and the associated entropy measures are tabulated in Table 5.

Table 5: Numerical values of degree-based and neighborhood degree sum-based topological indices and their respective entropy measures of Molnupiravir.

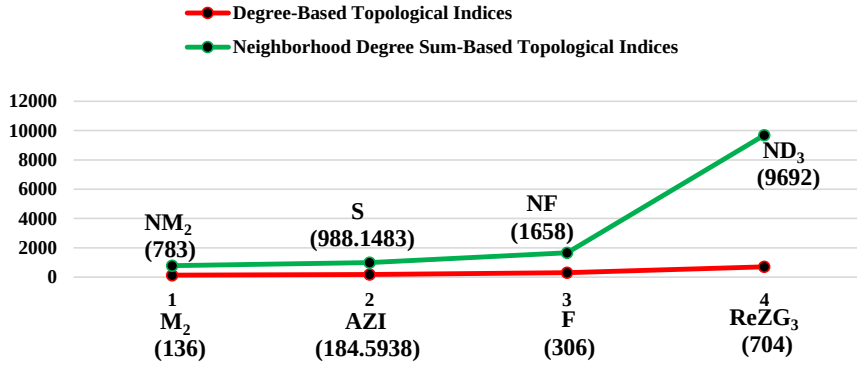
Degree-based		**Neighborhood Degree Sum-based**	
Topological Index	**Entropy Measures**	**Topological Index**	**Entropy Measures**
$M_1 = 116$	$E_{M_1} = 3.1623$	$NM_1 = 272$	$E_{NM_1} = 3.1545$
$M_2 = 136$	$E_{M_2} = 3.0916$	$NM_2 = 783$	$E_{NM_2} = 3.0811$
$^{m}M_2 = 5.1667$	$E_{^{m}M_2} = 3.0724$	$^{nm}M_2 = 0.9353$	$E_{^{nm}M_2} = 3.0350$
$ReZG_3 = 704$	$E_{ReZG_3} = 3.0211$	$ND_3 = 9692$	$E_{ND_3} = 2.9901$
$R_{-1/2} = 10.8454$	$E_{R_{-1/2}} = 3.1518$	$NR_{-1/2} = 4.5774$	$E_{NR_{-1/2}} = 2.9877$
$R_{1/2} = 55.8519$	$E_{R_{1/2}} = 3.1544$	$NR_{1/2} = 133.6166$	$E_{NR_{1/2}} = 3.1477$
$F = 306$	$E_F = 3.1362$	$NF = 1658$	$E_{NF} = 3.1017$
$SDD = 58$	$E_{SDD} = 3.1546$	$ND_5 = 52.3714$	$E_{ND_5} = 3.4990$
$H = 10.2667$	$E_H = 3.1606$	$NH = 4.4607$	$E_{NH} = 3.1496$
$ISI = 26.9667$	$E_{ISI} = 3.1443$	$NI = 65.6799$	$E_{NI} = 3.1470$
$AZI = 184.5938$	$E_{AZI} = 3.1026$	$S = 988.1483$	$E_S = 4.6389$

To display a better comparison between degree-based and related neighborhood degree sum-based topological indices of Molnupiravir, we partitioned the topological indices into two groups based on the range of their numerical values. These comparison plots of the topological indices of Molnupiravir are displayed in Figure 5. On the other hand, Figure 6 compares degree-based and neighborhood degree sum-based entropy measures for Molnupiravir.



(a)

Comparison between degree-based topological indices ($^{m}M_2$, H, $R_{-1/2}$, ISI, $R_{-1/2}$, SDD and M_1) and associated neighborhood degree sum-based topological indices of Molnupiravir.



(b)

Comparison between degree-based topological indices (M_2, AZI, F and $ReZG_3$) and associated neighborhood degree sum-based topological indices of Molnupiravir.

Figure 5: Comparison plots of the topological indices of Molnupiravir.

Figure 5 illustrates that there is a difference in the values of degree-based topological indices and their corresponding neighborhood degree sum-based topological indices. Figure 6 shows that degree-based and neighborhood degree sum-based entropy measures yield approximately equal values, except the entropy measures associated with Randić index ($\alpha = -1/2$), symmetric division degree index and augmented Zagreb index.

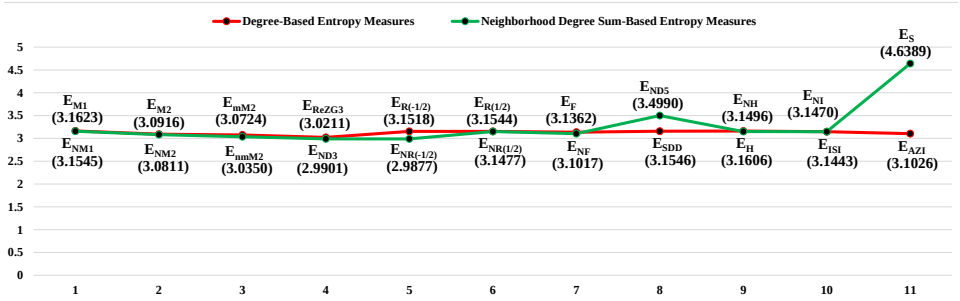


Figure 6: Comparison between degree-based and associated neighborhood degree sum-based entropy measures of Molnupiravir.

5 Conclusion

The first oral antiviral medication to show a perceptible reduction in hospitalization or mortality in cases of mild COVID-19 is Molnupiravir, which may prove to be a crucial tool in the fight against SARS-CoV-2. However, further research is required, as its significance in moderate to severe COVID-19 is debatable. In this work, we addressed the graph entropies associated with a new information function, based on Shannon's definition of entropy. We have evaluated the degree-based entropies and neighborhood degree sum-based entropies of the hydrogen-suppressed graph structure of the first oral anti-viral COVID-19 drug Molnupiravir, and shown the relationship among the different degree-based as well as neighborhood degree sum-based entropies for the drug. Figures 3 and 4 exhibit the graphical illustrations of both degree-based and neighborhood degree sum-based entropy measures, respectively which are arranged in increasing order. Our comparison analysis reveals that the neighborhood degree sum-based topological indices differ significantly from their corresponding degree-based topological indices. Whereas the degree sum-based and neighborhood degree sum-based entropy measures produce approximately similar numerical values, with the notable exceptions of Randić entropy ($\alpha = -1/2$), symmetric division degree entropy and augmented Zagreb entropy. The entropy measures obtained may aid researchers in predicting the physicochemical properties of Molnupiravir via quantitative structure-property relationship (QSPR) analysis for drug design and development.

Acknowledgment The authors (Shibsankar Das and Arti Kumari) are obliged to the Science and Engineering Research Board (SERB), Department of Science and Technology, Government of India, for financially supporting this work, through the SERB's research project sanction order number: EEQ/2022/000313, dated 20 January, 2023.

Author Contributions All the authors contributed equally.

Data Availability Statement The data used to support the findings of this study are included within article.

Disclosure Statement & Competing Interests No disclosure statement and potential conflict of interest was reported by the authors.

References

[1] Norah Almalki and Hafsah Tabassum. On K-Banhatti, Revan Indices and Entropy Measures of MgO (111) Nanosheets via Linear Regression. *Mathematics*, 12(4):561, 2024. doi:10.3390/math12040561.

[2] Zengqiang Chen, Matthias Dehmer, and Yongtang Shi. A note on distance-based graph entropies. *Entropy*, 16(10):5416–5427, 2014. doi:10.3390/e16105416.

[3] Yu-Ming Chu, K Julietraja, P Venugopal, Muhammad Kamran Siddiqui, and Savari Prabhu. Degree-and irregularity-based molecular descriptors for benzenoid systems. *The European Physical Journal Plus*, 136(1):1–17, 2021. doi:10.1140/epjp/s13360-020-01033-z.

[4] Shibsankar Das, Virendra Kumar, and Jayjit Barman. Geometric-quadratic and quadratic-geometric indices-based entropy measures of silicon carbide networks. *Silicon*, 17:75–91, 2024. doi:10.1007/s12633-024-03173-8.

[5] Shibsankar Das and Arti Kumari. Degree-based coindices of molnupiravir and its QSPR analysis with other COVID-19 drugs. *International Journal of Applied and Computational Mathematics*, 11(3):1–23, article number 109, 2025. doi:10.1007/s40819-025-01917-7.

[6] Shibsankar Das and Modhuleena Mandal. Deriving M-polynomial based topological descriptors of oral antiviral clinical drug Nirmatrelvir. *Scientific Annals of Computer Science*, 34(2):113–138, 2024. doi:10.47743/SACS.2024.2.113.

[7] Shibsankar Das, Shikha Rai, and Virendra Kumar. On topological indices of Molnupiravir and its QSPR modelling with some other antiviral drugs to treat COVID-19 patients. *Journal of Mathematical Chemistry*, 62(10):2581–2624, 2024. doi:10.1007/s10910-023-01518-z.

[8] Shibsankar Das, Shikha Rai, and Modhuleena Mandal. M-polynomial and correlated topological indices of antiviral drug Molnupiravir used as a therapy for COVID-19. *Polycyclic Aromatic Compounds*, 43(8):7027–7041, 2023. doi:10.1080/10406638.2022.2131854.

[9] Matthias Dehmer. Information processing in complex networks: Graph entropy and information functionals. *Applied Mathematics and Computation*, 201(1-2):82–94, 2008. doi:10.1016/j.amc.2007.12.010.

[10] Matthias Dehmer, Lavanya Sivakumar, and Kurt Varmuza. Uniquely discriminating molecular structures using novel eigenvalue-based descriptors. *MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY*, 67:147–172, 2012.

[11] Mohd Imran, Mandeep Kumar Arora, Syed Mohammed Basheeruddin Asdaq, Shah Alam Khan, Saleh I Alaqel, Mohammed Kanan Alshammari, Mohammed M Alshehri, Ahmed Subeh Alshrari, Alreshidi Mateq Ali, Ahmed Muteb Al-Shammeri, et al. Discovery, development, and patent trends on molnupiravir: A prospective oral treatment for COVID-19. *Molecules*, 26(19):5795, 2021. doi:10.3390/molecules26195795.

[12] Angélica Jayk Bernal, Monica M Gomes da Silva, Dany B Musungaie, Evgeniy Kovalchuk, Antonio Gonzalez, Virginia Delos Reyes, Alejandro Martín-Quirós, Yoseph Caraco, Angela Williams-Diaz, Michelle L Brown, et al. Molnupiravir for oral treatment of Covid-19 in nonhospitalized patients. *New England Journal of Medicine*, 386(6):509–520, 2022. doi:10.1056/NEJMoa2116044.

[13] K Julietraja, S Arul Amirtha Raja, and Ammar Alsinai. Neighbourhood Sum-Based Structural Analysis for Sodalite System.

Current Organic Synthesis, 22(4):548–555, 2025. doi:10.2174/0115701794320235240926054912.

[14] Konsalraj Julietraja, Padmanabhan Venugopal, Savari Prabhu, Arumugam Krishnan Arulmozhi, and Muhammad Kamran Siddiqui. Structural analysis of three types of PAHs using entropy measures. *Polycyclic Aromatic Compounds*, 42(7):4101–4131, 2022. doi:10.1080/10406638.2021.1884101.

[15] Florian Kabinger, Carina Stiller, Jana Schmitzová, Christian Dienemann, Goran Kokic, Hauke S Hillen, Claudia Höbartner, and Patrick Cramer. Mechanism of molnupiravir-induced SARS-CoV-2 mutagenesis. *Nature structural & molecular biology*, 28(9):740–746, 2021. doi:10.1038/s41594-021-00651-0.

[16] Virendra Kumar and Shibsankar Das. On Nirmala indices-based entropy measures of silicon carbide network. *Iranian Journal of Mathematical Chemistry*, 14(4):271–288, 2023. doi:10.22052/ijmc.2023.252742.1704.

[17] Virendra Kumar, Shibsankar Das, and Jayjit Barman. Neighborhood degree sum-based entropy measures of some silicon carbide networks. *Journal of Chemical Sciences*, Article in press.

[18] Cheng-Peng Li, Muhammad Kamran Siddiqui, Parvez Ali, Sana Javed, Mazhar Hussain, and Sadia Khalid. On analysis of entropy measures for titanium dioxide via rational curve fitting methods. *International Journal of Quantum Chemistry*, 122(23):e26996, 2022. doi:10.1002/qua.26996.

[19] Shazia Manzoor, Muhammad Kamran Siddiqui, and Sarfraz Ahmad. On entropy measures of polycyclic hydroxychloroquine used for novel coronavirus (COVID-19) treatment. *Polycyclic Aromatic Compounds*, 42(6):2947–2969, 2022. doi:10.1080/10406638.2020.1852289.

[20] Nicolas Rashevsky. Life, information theory, and topology. *Bulletin of Mathematical Biophysics*, 17:229–235, 1955. doi:10.1007/BF02477860.

[21] C. E. Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27(3):379–423, 1948. doi:10.1002/j.1538-7305.1948.tb01338.x.

[22] Awadhesh Kumar Singh, Akriti Singh, Ritu Singh, and Anoop Misra. Molnupiravir in COVID-19: A systematic review of literature. *Diabetes & Metabolic Syndrome: Clinical Research & Reviews*, 15(6):102329, 2021. doi:10.1016/j.dsx.2021.102329.

[23] Melaiyur Sankarraman Srinivasan and Ranjan Helen. Novel M-Polynomials for computing graph invariants of certain drugs: Targeting COVID-19 and Omicron. *Letters in Applied NanoBioScience*, 13(4):1–23, 2024. doi:10.33263/LIANBS134.178.

[24] William Tamilarasi and Bommahalli Jayaraman Balamurugan. ADMET and quantitative structure property relationship analysis of anti-Covid drugs against omicron variant with some degree-based topological indices. *International Journal of Quantum Chemistry*, 122(20):e26967, 2022. doi:10.1002/qua.26967.

[25] National Center for Biotechnology Information. PubChem compound summary, Accessed on May 30, 2024. URL: https://pubchem.ncbi.nlm.nih.gov/compound/eidd-2801#section=Structures.

[26] World Health Organization. Emergencies, Accessed on May 30, 2024. URL: https://www.who.int/europe/emergencies/situations/covid-19.

[27] Hua Wagner, Stephan; Wang. *Introduction to chemical graph theory*. Discrete mathematics and its applications. CRC Press, 2019.

[28] Douglas B. West. *Introduction to graph theory*. Prentice Hall, Upper Saddle River, 2nd edition, 2000.

[29] Jun Yang, Julietraja Konsalraj, and Arul Amirtha Raja S. Neighbourhood sum degree-based indices and entropy measures for certain family of graphene molecules. *Molecules*, 28(1):168, 2022. doi:10.3390/molecules28010168.